

On the self-consistent spin-wave theory of two-dimensional magnets with impurities

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The self-consistent spin-wave theory is applied to investigate the magnetization distribution around the impurity in isotropic and easy-axis two-dimensional ferro- and antiferromagnets. The temperature dependences of host magnetization disturbance and impurity magnetization are calculated. The short-range order in the isotropic case is investigated. Importance of dynamic and kinematic interactions of spin waves is demonstrated.

I. INTRODUCTION

In connection with extensive investigations of copper-oxide based superconductors, great attention is paid last time to studying magnetism of low-dimensional systems. Of particular interest is the problem of non-magnetic impurities in magnetic hosts. Numerous experimental results (see, e.g., [1–3]) demonstrate that even small amount of substitution impurities (Zn, Fe etc.) in CuO_2 planes may influence strongly magnetic properties, e.g. lead to strong suppression of host magnetization. These facts have stimulated a number of theoretical works (see, e.g., [2–5]). In particular, the impurity problem for isotropic two-dimensional (2D) antiferromagnets at $T = 0$ was investigated by the standard spin-wave theory [5]. However, the detailed consideration of the finite temperature situation is absent. Moreover, the usual spin-wave theory is obviously inapplicable, since this does not take into account adequately the short-range magnetic order which is a characteristic feature of low-dimensional magnets.

On the other hand, the impurity problem for three-dimensional (3D) magnets was investigated within the standard spin-wave theory (see, e.g. [6]). It was established that in the case of a weakly coupled magnetic impurity in a ferromagnet the standard spin-wave approximation is insufficient already at $T \sim T_{imp}$ where $T_{imp} \ll T_C$ is the energy of impurity-host coupling. Inclusion of dynamic and kinematic interaction of spin waves within the Tyablikov approximation [6] leads in this case to occurrence of an anomalous temperature dependence of impurity magnetization. Therefore it is interesting to investigate the impurity problem for two-dimensional (2D) systems, such as ferro- and antiferromagnets (FM and AFM) with small anisotropy or interlayer coupling, which are required to produce a finite value of the magnetic ordering temperature T_M .

In the present paper we consider weakly anisotropic 2D impurity magnetic crystals with the use of the self-

consistent spin-wave theory (SSWT). This theory was developed to describe thermodynamics of 2D systems [7,8], and also successfully applied to quasi-2D [10,11] and weakly anisotropic 2D magnets [11]. An important advantage of SSWT in comparison with the usual spin-wave theory is a qualitatively correct description of the strong short-range order above T_M . Besides that, introducing slave fermions [12] into SSWT allows to take into account kinematic interactions of spin waves and describe systems with not too low T_M values. In the following sections we treat the cases of different signs of exchange interactions in the host and between host and impurity.

II. FERROMAGNETIC IMPURITY IN FERROMAGNETIC HOST

The Heisenberg Hamiltonian of a FM crystal with a quadratic lattice, containing a ferromagnetically coupled impurity at the site $i = 0$, reads

$$\mathcal{H} = -\frac{1}{2} \sum_{ij} J_{ij} \mathbf{S}_i \mathbf{S}_j + \mathcal{H}_A - H \sum_i S_i^z \quad (1)$$

where

$$\mathcal{H}_A = -D \sum_i (S_i^z)^2 - \frac{1}{2} \sum_{ij} \eta_{ij} S_i^z S_j^z$$

is the Hamiltonian of the easy-axis anisotropy, H is external magnetic field. In the nearest-neighbor approximation the non-zero exchange integrals are

$$J_{i,i+\delta} = \begin{cases} J', & i = 0 \text{ or } i + \delta = 0 \\ J, & i, i + \delta \neq 0 \end{cases} \quad (2)$$

where δ denotes nearest neighbors, $J > 0$, $J' > 0$.

Following to Ref. [11] we use in the FM case for $i \neq 0$ the representation [12]

$$\begin{aligned} S_i^+ &= \sqrt{2S} a_i, \quad S_i^z = S - a_i^\dagger a_i - (2S+1) c_i^\dagger c_i \\ S_i^- &= \sqrt{2S} (a_i^\dagger - \frac{1}{2S} a_i^\dagger a_i^\dagger a_i) - \frac{2(2S+1)}{\sqrt{2S}} a_i^\dagger c_i^\dagger c_i \end{aligned} \quad (3)$$

where a_i^\dagger, a_i are the Bose ideal magnon operators and c_i^\dagger, c_i are the auxiliary Fermi operators at the site i which take into account the kinematic interaction of spin waves. For $i = 0$ one has to replace in (3) $S \rightarrow S'$ with S' the impurity spin. Note that in the paper [8] only the Bose operators were introduced.

To satisfy the condition $\overline{S}_i(H=0) = 0$ in the paramagnetic phase we introduce the Lagrange multipliers μ_i at

each lattice site, which corresponds to the constraint of the magnon occupation number at $T > T_C$. These multipliers play the role of a local “chemical potential” for the boson-fermion systems. Introducing μ_i permits to correct the drawback of the standard spin-wave theory which is inapplicable at $T > T_C$ since the magnetization formally becomes negative. Unlike the approach of Ref. [8], we do not assume *ad hoc* the condition $\bar{S} = 0$ in the ordered phase where we have $\mu_i = 0$. Thus in our approach the magnon number is not conserved at $T < T_C$ and the Bose condensation [8] does not take place. However, it may be shown that the results of both approaches are identical at low temperatures where kinematical interactions are small.

Further we perform decouplings of the quartic forms which occur after substituting (3) into (1). Introducing the averages

$$\xi_{i,i+\delta} = \bar{S}_{i+\delta} + \langle a_i^\dagger a_{i+\delta} \rangle \quad (4)$$

we derive the quadratic Hamiltonian of the mean-field approximation

$$\mathcal{H} = \sum_{i\delta} \xi_{i,i+\delta} J_{i,i+\delta} \left[a_i^\dagger a_i - a_{i+\delta}^\dagger a_{i+\delta} + (2S+1)c_i^\dagger c_i \right] \quad (5) \\ + \sum_i (H - \mu_i) \left[a_i^\dagger a_i + (2S+1)c_i^\dagger c_i \right] + \mathcal{H}_A$$

This Hamiltonian differs from that of the standard spin-wave theory in two points. First, the averages $\xi_{i,i+\delta}$ are introduced which take into account the dynamical interaction of spin waves in the lowest Born approximation (see below). Second, the Fermi operators enter to account the kinematic interactions of the spin-waves.

Following to Ref. [13], we treat the influence of the magnetic anisotropy by neglecting quartic forms in \mathcal{H}_A to obtain

$$\mathcal{H}_A = -H_A \sum_i S_i^z \\ = -H_A \sum_i \left[S - a_i^\dagger a_i - (2S+1)c_i^\dagger c_i \right]$$

with the anisotropy field H_A

$$H_A = (2S-1)D + S \sum_{\delta} \eta_{i,i+\delta} \quad (6)$$

Note that effects of the true magnetic field H and the field H_A are different in the paramagnetic phase since chemical potentials μ_i are calculated at $H = 0$, not $H_A = 0$. Thus the field H yields a finite magnetization at any temperatures, whereas the field H_A induces a slight shift of T_C only. Thus the field H_A describes correctly the effect of the easy-axis anisotropy. In the limit $H_A \ll J$ under consideration effects of single-site and two-site anisotropy are the same, although concrete expressions for the field H_A in (6) are different.

For an ideal crystal $\xi_{i,i+\delta}, \mu_i$ do not depend on i and the diagonalization of the Hamiltonian (5) is easily performed [8,11]. At the same time, for the impurity system this is a complicated task since the unknown dependence $\xi_{i,i+\delta}, \mu_i$ which is to be determined self-consistently. However, as follows from the below calculations, $\xi_{i,i+\delta}$ and μ_i practically coincide with the corresponding quantities for the host, ξ_M and μ , except for nearest neighbors of impurity. Also in the FM phase $\xi_{i,i+\delta}$ as a function of i varies slower than the magnetization, and $\mu_i = 0$. Therefore we may put in (5)

$$\xi_{i,i+\delta} = \begin{cases} \xi, & i = 0 \\ \xi', & i + \delta = 0 \\ \xi_M, & \text{otherwise} \end{cases}, \quad \mu_i - \mu = \begin{cases} \delta\mu_0, & i = 0 \\ \delta\mu_1, & i + \delta = 0 \\ 0, & \text{otherwise} \end{cases} \quad (7)$$

Note that $\xi \neq \xi'$ because of non-Hermiticity of the representation (3). Taking into account (3) the spin correlation function of impurity spin with its nearest neighbors has the form

$$K \equiv |\langle \mathbf{S}_0 \mathbf{S}_\delta \rangle| = \xi \xi' \quad (8)$$

Under the approximation 7 the Hamiltonian (5) takes the form

$$\mathcal{H} = \mathcal{H}_0 + V \quad (9)$$

where

$$\mathcal{H}_0 = J\xi_M \sum_{i\delta} \left[a_i^\dagger a_i - a_{i+\delta}^\dagger a_{i+\delta} + (2S+1)c_i^\dagger c_i \right] \quad (10) \\ + (H_A + H - \mu) \sum_i \left[a_i^\dagger a_i + (2S+1)c_i^\dagger c_i \right]$$

is the standard SSWT Hamiltonian without impurities [8,11] and

$$V = (J'\xi - J\xi_M) \sum_{\delta} \left[a_0^\dagger a_0 - a_\delta^\dagger a_\delta + (2S'+1)c_0^\dagger c_0 \right] \quad (11) \\ + (J'\xi' - J\xi_M) \sum_{\delta} \left[a_\delta^\dagger a_\delta - a_0^\dagger a_0 + (2S+1)c_\delta^\dagger c_\delta \right] \\ + \delta\mu_0 b_0^\dagger b_0 + \delta\mu_1 \sum_{\delta} a_\delta^\dagger a_\delta$$

To diagonalize \mathcal{H} we introduce the Green's functions

$$G_{ij}^0(\omega) = \ll a_j | a_i^\dagger \gg_\omega^0 = \sum_{\mathbf{q}} \frac{1}{\omega - E_{\mathbf{q}}} e^{i\mathbf{q}(\mathbf{R}_i - \mathbf{R}_j)} \quad (12)$$

$$G_{ij}(\omega) = \ll a_j | a_i^\dagger \gg_\omega$$

where the index 0 means that statistical averages are calculated with H_0 ,

$$E_{\mathbf{q}} = \xi_M(J_0 - J_{\mathbf{q}}) + H_A + H - \mu, \quad J_{\mathbf{q}} = 2J(\cos q_x + \cos q_y)$$

In the limit $R \gg 1$ we find by using the saddle point approximation (see, e.g., [6])

$$G_{0R}^0(\omega) \sim \begin{cases} \exp(i\sqrt{\omega/J\xi_M}R)/\omega^{1/4}R^{1/2} & 1 \ll (\omega/J)^{1/2}R, \omega \ll 1 \\ -\ln(\omega/J) & (\omega/J)^{1/2}R \ll 1 \end{cases} \quad (13)$$

The perturbation V can be written in the matrix form

$$V = \sum_{i,j=0}^4 V_{ij}a_i^\dagger a_j + \sum_{i=0}^4 R_i c_i^\dagger c_i \quad (14)$$

where the indices i, j enumerate the impurity site and its four nearest neighbors. From (11) we have

$$V = \begin{pmatrix} 4\varepsilon & \gamma & \gamma & \gamma & \gamma \\ \gamma' & \rho & 0 & 0 & 0 \\ \gamma' & 0 & \rho & 0 & 0 \\ \gamma' & 0 & 0 & \rho & 0 \\ \gamma' & 0 & 0 & 0 & \rho \end{pmatrix}, \quad R = (2S+1) \begin{pmatrix} 4\varepsilon \\ \rho \\ \rho \\ \rho \\ \rho \end{pmatrix} \quad (15)$$

$$\begin{aligned} \gamma' &= J'\xi - J\xi_M, \quad \varepsilon = \gamma' + \delta\mu_0/4, \\ \gamma &= J'\xi' - J\xi_M, \quad \rho = \gamma + \delta\mu_1 \end{aligned}$$

Then we have the expression for the perturbed Green's function [6]:

$$\tilde{G}(\omega) = [1 - \tilde{G}^0(\omega)V]^{-1}\tilde{G}^0(\omega) \quad (16)$$

where $\tilde{G}(\omega)$, $\tilde{G}^0(\omega)$ are submatrices of matrices $G_{ij}(\omega)$, $G_{ij}^0(\omega)$ with $i, j = 0 \dots 4$. Further we calculate the matrix G from (16) and the averages $\langle a_i^\dagger a_j \rangle$ from the spectral representation. Then we derive from (3), (7) the system of self-consistency equations

$$\begin{aligned} \xi &= \bar{S}_1 + \int_{-\infty}^{+\infty} \frac{d\omega}{\pi} N(\omega) \text{Im} \tilde{G}_{10}(\omega), \\ \xi' &= \bar{S}_0 + \int_{-\infty}^{+\infty} \frac{d\omega}{\pi} N(\omega) \text{Im} \tilde{G}_{01}(\omega) \end{aligned} \quad (17)$$

where $N(\omega) = 1/(\exp(\omega/T) - 1)$ is the Bose distribution function. The integration region in (17) is in fact $\alpha \leq \omega \leq 2\xi_M J_0 + \alpha$, $\alpha = H_A + H - \mu$. The expressions for the site magnetizations take the form

$$\begin{aligned} \bar{S}_0 &= S' - \int_{-\infty}^{+\infty} \frac{d\omega}{\pi} N(\omega) \text{Im} \tilde{G}_{00}(\omega) + (2S' + 1)N(E_0) \\ \bar{S}_1 &= S - \int_{-\infty}^{+\infty} \frac{d\omega}{\pi} N(\omega) \text{Im} \tilde{G}_{11}(\omega) + (2S + 1)N(E_1) \end{aligned} \quad (18)$$

where $E_i = (2S_i + 1)J\xi_M + \alpha - \delta\mu_i$ is the fermion energy at the site i .

In the case of the pure system ($V = 0$) we have $\tilde{G} = \tilde{G}^0$ and the values \bar{S}_i , $\xi_{i,i+\delta}$, μ_i are independent of i , so that the system of equations (17), (18) reduces to

$$\xi = \xi' = \bar{S} + \frac{1}{J_0} \sum_{\mathbf{k}} J_{\mathbf{k}} N(E_{\mathbf{k}}) \quad (19)$$

$$\bar{S} = S - \sum_{\mathbf{k}} N(E_{\mathbf{k}}) + (2S + 1)N(E_f)$$

where $E_f = (2S + 1)J\xi_M + \alpha$. One can see that ξ depends on temperature due to dynamic magnon-magnon interactions; at low temperatures the corrections are proportional to $T^{5/2}$, as well as in the Dyson's theory [14].

The results of numerical solution of the equations (19) at different values of H_A are shown on Fig.1. The results of numerical solution of Eqs. (19) for different H_A are shown on Fig.1. While the magnetization is strongly dependent from the value of H_A , the dependence $\xi(T)$ is the same to calculation accuracy at an arbitrary $H_A/J \ll 1$. This dependence coincide with those for the ferromagnet in earlier variants of SSWT [8] at low temperatures. However, at $T \sim J$ the short-range order parameter ξ demonstrates a sharp decrease rather than vanishing. Thus introducing the Fermi operators removes the unphysical transition with vanishing of short-range order parameter. At finite values of H_A the value of the Curie temperature is finite. At small $H_A \ll J$ we have (cf. [11])

$$T_C = \begin{cases} 4\pi JS^2 / \ln(T/H_A) & 1 \ll \ln(J/H_A) \ll 2\pi S \\ 4\pi JS^2 / \ln(\pi^2 J/H_A) & \ln(J/H_A) \gg 2\pi S \end{cases} \quad (20)$$

Now we turn to the consideration of the impurity system. The results of numerical calculations of magnetizations \bar{S}_0, \bar{S}_1 vs. temperature according to (17), (18) in the zero magnetic field are presented in Figs 2,3. In Fig.2 the results of the standard spin-wave theory (SW) which correspond, in our notations, to $\xi_M = \xi = \xi' = S$, fermion occupation numbers $N(E_i)$ being replaced by zero, and the spin-wave theory with introducing fermions (SWF) are also presented for comparison. We see that the impurity magnetization has an anomalous behavior at temperatures $T \sim J'$. On the inset on Fig.2 this dependence is shown at a different H_A/J , J'/J . The sharp decrease of impurity-site magnetization at $T \sim J'$ can be easily obtained already in the simple mean-field approximation, however the detailed description of the this behavior requires a more complicated methods. The standard spin-wave, as well as the SWF solution do not show this anomaly, so we can conclude that it is caused by both dynamic and kinematic interactions of spin waves. The situation is similar to the 3D case where using the Tyablikov approximation results in a strong modification of the magnetization behavior in this temperature interval [6].

In the ground state the disturbance of magnetization is localized at the impurity site and equals to $S' - S$. To

calculate the magnetization distribution around impurity at finite temperatures we need the full matrix G . It may be shown (see, e.g., [6]) that the latter quantity is given by

$$G = G^0 + \tilde{G}^{0N} V \frac{1}{1 - \tilde{G}^{0N} V} \tilde{G}^{N0} \quad (21)$$

where \tilde{G}^{0N} is the submatrix of G_{ij}^0 with $i = 0..4$, $j = 0..N$, and \tilde{G}^{N0} is the conjugated matrix. Using (21) we can find the averages needed. The results of numerical calculation of magnetization disturbance for different values of J'/J , H_A/J are presented in Fig.4. One can see that at $R > 0$ all results are practically the same, this takes place also in the limiting case with $J' = 0$ (or in the case of vacancy with $S' = 0$). One can see that the change of magnetization around the impurity rapidly decreases with increasing distance from the impurity site, so that the magnetization disturbance practically vanishes at the distance of 4 coordination spheres.

In the 2D isotropic magnets where the long-range order at finite temperatures is absent we have to treat the short-range order parameters ξ_{ij} only. The chemical-potential corrections $\delta\mu_i$, $i = 0, 1$ are defined from the condition

$$\begin{aligned} & \left[S - \langle a_i^\dagger a_i \rangle - (2S+1) \langle c_i^\dagger c_i \rangle \right]_{H=0} \\ &= S - \int_{-\infty}^{+\infty} \frac{d\omega}{\pi} N(\omega) \text{Im} \tilde{G}_{ii}(\omega) \Big|_{H=0} \\ &+ (2S+1) N(E_i) \Big|_{H=0} = 0 \end{aligned} \quad (22)$$

In zero magnetic field the solution to eqs (17), (18), (22) is not unique. The absence of the unique solution in the paramagnetic phase is apparently the shortcoming of our approach. Since at small values of H the solution is unique, it is natural to take H to be small, but finite (in numerical calculations we have taken $H = 0.005J$). Although the site magnetizations are changed strongly with changing H (the susceptibility $\chi = \partial \bar{S} / \partial H$ is divergent near $T = 0$), it may be checked analytically that the derivative $\partial \xi / \partial H$ remains finite at $H \rightarrow 0$, so that the values of ξ, ξ' weakly depend of H . This may be verified also by numerical calculations.

The numerical procedure is as follows. To find the short-range order parameters ξ, ξ' we solve the system of equations (17). At each iteration for given values of ξ, ξ' , the corrections to the chemical potential $\delta\mu_0, \delta\mu_1$ and magnetizations \bar{S}_0, \bar{S}_1 are determined from eqs (22) and (18), respectively. Results of numerical calculation of the short-range order parameters ξ, ξ' and correlation function K for the case of a weakly coupled impurity for the 2D ferromagnet are shown in Fig.5. One can see that, owing to sharp decrease of ξ' , the correlations between the impurity site and its nearest neighbors decrease with temperature more rapidly than those in an ideal crystal.

III. ANTIFERROMAGNETIC IMPURITY IN FERROMAGNETIC HOST

Further we consider an AFM impurity in FM host ($J > 0$, $J' < 0$ in 2). After passing to the local coordinate system at the impurity site, we have to use the representation

$$\begin{aligned} S_0^+ &= \sqrt{2S'} b_0^\dagger, \quad S_0^z = -S' + b_0^\dagger b_0 + (2S' + 1) d_0^\dagger d_0 \\ S_0^- &= \sqrt{2S'} (b_0 - \frac{1}{2S'} b_0^\dagger b_0 b_0) - 2 \frac{2S' + 1}{2S'} d_0^\dagger d_0 b_0 \end{aligned} \quad (23)$$

where b_0^\dagger, b_0 are the Bose operators, d_0^\dagger, d_0 are the Fermi operators. Then, in the mean-field approximation, the Hamiltonian (1) takes the form

$$\begin{aligned} \mathcal{H} &= \frac{1}{2} J \sum_{i, i+\delta \neq 0} \xi_{i, i+\delta} \left[a_i^\dagger a_i - a_{i+\delta}^\dagger a_i + (2S+1) b_i^\dagger b_i \right] \\ &+ |J'| \sum_{\delta} \left\{ \xi \left[a_\delta^\dagger a_\delta - b_0 a_\delta + (2S' + 1) b_\delta^\dagger b_\delta \right] \right. \\ &\quad \left. + \xi' \left[b_0^\dagger b_0 - b_0^\dagger a_\delta^\dagger + (2S' + 1) c_0^\dagger c_0 \right] \right\} \\ &+ \sum_{i \neq 0} (H_A + H - \mu_i) \left[a_i^\dagger a_i + (2S+1) b_i^\dagger b_i \right] \\ &+ (H_A + H - \mu_0) \left[b_0^\dagger b_0 + (2S' + 1) c_0^\dagger c_0 \right] \end{aligned} \quad (24)$$

where

$$\begin{aligned} \xi &= \bar{S}_0 + \langle d_0^\dagger a_\delta^\dagger \rangle \\ \xi' &= \bar{S}_1 + \langle a_\delta d_0 \rangle \end{aligned}$$

As in ferromagnetic case, we use the approximation $\xi_{i, i+\delta} \simeq \xi_M$ ($i, i+\delta \neq 0$). To diagonalize (24) we introduce, following to [6], the “hole” creation and annihilation operators a_0^\dagger, a_0 by the canonical transformation

$$a_0 = d_0^\dagger, \quad a_0^\dagger = -d_0$$

As well as in the case of FM impurity, we use the approximation (7). We introduce also the Green’s functions (12) and represent the Hamiltonian as (9) with the parameters of the matrix V (15)

$$\begin{aligned} \gamma' &= -J'\xi + J\xi_M, \quad \varepsilon = -J'\xi - J\xi_M + \delta\mu_0/4, \\ \gamma &= J'\xi' + J\xi_M, \quad \rho = J'\xi - J\xi_M + \delta\mu_1 \end{aligned}$$

Then we have the same equation (16) for the full Green’s function as in the case of FM impurity, the self-consistency equations also has the same form (17), (18). Unlike the FM impurity case, the full Green’s function has a pole at $\omega = -\omega_0 < 0$ [6]. To take into account the contribution from this pole to the averages needed we deform the integration path in the spectral representation for the Green’s function in the complex plane:

$$\begin{aligned} \langle a_i^\dagger a_i \rangle &= \frac{1}{\pi} \int_{-\infty}^{+\infty} d\omega N(\omega) \text{Im} G_{ij}(\omega) \\ &= \int_C \frac{d\omega}{2\pi i} N(\omega) G_{ij}(\omega) - T G_{ij}(0) \end{aligned} \quad (25)$$

The contour C is selected in such a way that all singularities of $G(\omega)$ lie inside C , but all the frequencies $\omega_n = 2\pi nT$ ($n \neq 0$) lie outside it. The last term in (25) corresponds to the contribution from $\omega = 0$ which is to be subtracted explicitly.

Results of numerical solution of Eqs. (17), (18) with using of (25) for different values of impurity-host coupling and $H = 0$ are presented in Figs.6,7.

The AFM impurity induces the disturbance of host magnetization already at $T = 0$. Using the sum rule

$$\pi \sum_i \text{Im} [G_{ii}(\omega + i\delta) - G_{ii}^0(\omega + i\delta)] = \frac{\partial}{\partial \omega} \text{Im} \ln \det[1 - G_0(\omega)V] \quad \text{where} \quad (26)$$

which follows from (21) and taking into account that $\det[1 - G_0(\omega)V]$ has a zero at $\omega = -\omega_0$ we obtain

$$\langle b_0^\dagger b_0 \rangle_{T=0} = \sum_{i>0} \langle a_i^\dagger a_i \rangle_{T=0} \quad (27)$$

so that the total disturbance of magnetization equals to $S + S'$ [6]. The distribution of magnetization around the impurity site is shown in Fig. 8. At large R the contribution from the pole $\omega = -\omega_0$ gives main contribution to the magnetization disturbance which is proportional to $\exp(-R\sqrt{\omega_0/J})/R$ and differs from that in the 3D case [6] by preexponential factor only.

IV. THE CASE OF AN ANTIFERROMAGNETIC HOST

Now we consider an antiferromagnet with the Hamiltonian

$$\mathcal{H} = -\frac{1}{2} \sum_{ij} J_{ij} \mathbf{S}_i \mathbf{S}_j + \mathcal{H}_A + H_{\mathbf{Q}} \sum_i e^{i\mathbf{Q}\mathbf{R}_i} S_i^z$$

with $J_{ij} < 0$, $\eta_{ij} < 0$, $\mathbf{Q} = (\pi, \pi)$, $H_{\mathbf{Q}}$ is the staggered magnetic field. In the case of two sublattices A, B and for the antiferromagnetically coupled impurity spin in the A sublattice we have to use the representation

$$\begin{aligned} S_i^+ &= \sqrt{2S} a_i, \quad S_i^z = S - a_i^\dagger a_i - (2S+1) c_i^\dagger c_i \\ S_i^- &= \sqrt{2S} (a_i^\dagger - \frac{1}{2S} a_i^\dagger a_i^\dagger a_i) - \frac{2(2S+1)}{2S} a_i^\dagger c_i^\dagger c_i \end{aligned} \quad (28)$$

for $i \in A$ and

$$\begin{aligned} S_i^+ &= \sqrt{2S} b_i^\dagger, \quad S_i^z = -S + b_i^\dagger b_i + (2S+1) d_i^\dagger d_i \\ S_i^- &= \sqrt{2S} (b_i - \frac{1}{2S} b_i^\dagger b_i b_i) - \frac{2(2S+1)}{2S} d_i^\dagger d_i b_i \end{aligned} \quad (29)$$

for $i \in B$ where a_i^\dagger, a_i and b_i^\dagger, b_i are the Bose operators, c_i^\dagger, c_i and d_i^\dagger, d_i are the Fermi operators. After standard decoupling the Hamiltonian takes the form

$$\begin{aligned} \mathcal{H} &= \sum_{i \in A, \delta} |J_{i,i+\delta}| \xi_{i,i+\delta} [a_i^\dagger a_i - b_{i+\delta} a_i + (2S+1) c_i^\dagger c_i] \\ &+ \sum_{i \in B, \delta} |J_{i,i+\delta}| \tilde{\xi}_{i,i+\delta} [b_{i+\delta}^\dagger b_{i+\delta} - b_{i+\delta}^\dagger a_i^\dagger + (2S+1) c_i^\dagger c_i] \\ &+ \sum_{i \in A} (H_A + H - \mu_i) [a_i^\dagger a_i + (2S+1) c_i^\dagger c_i] \\ &+ \sum_{i \in B} (H_A + H - \mu_i) [b_i^\dagger b_i + (2S+1) d_i^\dagger d_i] \end{aligned} \quad (30)$$

$$H_A = (2S-1)D + S \sum_i |\eta_{i,i+\delta}| \quad (31)$$

and

$$\xi_{i,i+\delta} = \bar{S}_{i+\delta} + \langle b_{i+\delta}^\dagger a_i^\dagger \rangle, \quad \tilde{\xi}_{i,i+\delta} = \bar{S}_i + \langle a_i b_{i+\delta} \rangle \quad (32)$$

For the correlation function K we have the same expression (8) as in the FM case with $\xi = \xi_{01}, \xi' = \tilde{\xi}_{01}$. To diagonalize (30) we introduce the operators

$$A_i = \begin{cases} a_i & i \in A \\ b_i^\dagger & i \in B \end{cases}$$

and the Green's functions:

$$\hat{G}_{ij}^0(\omega) = \ll A_i | A_j^\dagger \gg_\omega = G_{ij}^0(\Omega) \times \begin{cases} r, & i, j \in A \\ r^{-1}, & i, j \in B \\ 1, & \text{otherwise} \end{cases} \quad (33)$$

where

$$\begin{aligned} r &= \left(\frac{\lambda + \omega}{\lambda - \omega} \right)^{1/2}, \quad \Omega = \lambda - \sqrt{\lambda^2 - \omega^2}, \\ \lambda &= |J_0| \xi_M + H_A + H - \mu \end{aligned}$$

Using the approximation (7) we get the same expression for the Green's function (16) with $\tilde{G}^0(\omega)$ being the 5×5 submatrix of $\hat{G}_{ij}^0(\omega)$, and analogously for $\tilde{G}(\omega)$. In this designations the self-consistent equations for the site magnetizations and short-range order parameters has the same forms as in FM case (18), (17). In the case of the pure system we now have $\hat{G} = \hat{G}_0$ so that

$$\xi = \xi' = \bar{S} + \frac{1}{2J_0} \sum_{\mathbf{k}} \frac{\xi J_{\mathbf{k}}^2}{E_{\mathbf{k}}^{\text{AF}}} \coth \frac{E_{\mathbf{k}}^{\text{AF}}}{2T}$$

$$\bar{S} = S - \sum_{\mathbf{k}} \frac{\xi J_{\mathbf{k}}}{2E_{\mathbf{k}}^{\text{AF}}} \coth \frac{E_{\mathbf{k}}^{\text{AF}}}{2T} + (2S+1)N(E_f)$$

where

$$E_{\mathbf{k}}^{\text{AF}} = \sqrt{(|J_0|\xi_M + \alpha)^2 - (J_{\mathbf{k}}\xi_M)^2}$$

The results of numerical calculations for the AFM impurity system case are shown and compared with those for the FM case in Fig.9. In the case of an impurity spin, which is weakly coupled to the host, the behavior of magnetization in AFM and FM situations is very close, except for the region near the magnetic ordering temperature ($T_N > T_C$ because of quantum fluctuations). At the same time, the nearest-neighbor magnetizations are strongly different and demonstrate a behavior, typical for the corresponding hosts. One can also see that SSWT leads to unambiguous result at low T , where the impurity magnetization turns out to be greater than the host one. The difference between magnetizations of impurity and host increases with lowering value of J'/J and decreases with increasing temperature. Thus SSWT predicts strong influence of quantum fluctuations on magnetization in the case of weakly magnetic impurities.

The results of calculating the short-range order parameters ξ, ξ' and the correlation function K in the isotropic case $H_A = 0$ are presented in Fig. 10. We use the same procedure as in the FM case. The parameter ξ has a non-monotonic temperature dependence. At the same time, the temperature dependence of the correlation function of the impurity spin with its nearest neighbors is monotonic and more rapid than that for correlation functions between spins in the host.

To calculate the total magnetization disturbance we use the sum rule for the Green's functions (33)

$$\pi \sum_i (-1)^i \text{Im} \left[\hat{G}_{ii}(\omega + i\delta) - \hat{G}_{ii}^0(\omega + i\delta) \right] = \frac{\partial}{\partial \omega} \text{Im} \ln \det[1 - \hat{G}^0(\omega + i\delta)V] \quad (34)$$

Since $\det(1 - \hat{G}^0 V)$ has no zeros at $\omega < 0$, we obtain at $T = 0$

$$\delta M = S' - S - \frac{1}{\pi} \text{Im} \ln \det(1 - \hat{G}^0 V) \Big|_{-\infty}^0 = S' - S \quad (35)$$

This result is valid also for a vacancy if we put $S' = 0$. For a ferromagnetically coupled impurity we have to replace in (35) $S' \rightarrow -S'$.

The distribution of magnetization around impurity in the ground state of a 2D isotropic antiferromagnet is shown in Fig.11. The magnetization of each sublattice decreases, so that corrections to the host magnetization

have alternating signs. The values of sublattice magnetization disturbance are close to those in the spin-wave theory [5]. At large R , main contribution to the disturbance of sublattice magnetization comes from frequencies $\omega \ll J$. Expanding (21), (33) up to first order in ω/J we derive

$$\delta < A_0^\dagger A_i > \sim 1/R_i^3 \quad (36)$$

Note that in the 3D case this quantity demonstrates a more rapid decrease $1/R^4$, which may be obtained in the same manner.

V. CONCLUSIONS

To conclude, we have investigated 2D magnets with impurities for different signs of exchange integrals within the framework of self-consistent spin-wave theory [7,8]. This theory permits to calculate both magnetization distribution and the correlation functions (short-range order parameters). For $T = 0$ modifications of the results of the standard spin-wave theory are small. At the same time, for finite temperatures, corrections owing to dynamic and kinematic interactions of spin waves turn out to be important. It should be stressed that despite the absence of long-range order in the isotropic 2D magnets at $T > 0$, the temperature dependence of the impurity-host correlation function K (8) is similar to that in the 3D case, although in the latter case main contribution to K equals to $\bar{S}_0 \bar{S}_\delta$.

The distribution of magnetization in the ground state was investigated in detail. In the nearest-neighbor approximation considered, the host magnetization disturbance decreases rapidly with distance from impurity, and the total change of magnetic moment equals to $-S \pm S'$ depending on the sign of J' . More interesting situations occur in the case of the long-range exchange. So, in the case of FM impurity in the FM host with sufficiently strong negative next-nearest impurity-host exchange J'' , the total magnetization change equals

$$\delta M = S' - S - 2z_2 S \quad (37)$$

with z_2 the corresponding coordination number. In the case of FM impurity in the AFM host with large positive J'' we have

$$\delta M = S' - S + 2z_2 S. \quad (38)$$

It would be of interest also to investigate the problem of a current carrier in the AFM host within a similar approach (e.g., within the $t - J$ model, cf. [7]).

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FIGURE CAPTIONS.

Fig.1 The temperature dependences of the magnetization for the pure 2D ferromagnet with $S = 1/2$, $H_A/J = 10^{-2}$ (solid line), $H_A/J = 10^{-3}$ (dashed line) and short-range order parameter ξ (dot-dashed line which is the same for all three cases: $H_A/J = 0, 10^{-3}, 10^{-2}$).

Fig.2 The temperature dependence of the magnetizations for impurity site \bar{S}_0 , and for nearest-neighbor sites \bar{S}_1 ($S = S' = 1/2$, $H_A/J = 10^{-3}$, $J'/J = 0.15$). The results of the magnetization for the impurity site in the standard (non-self-consistent) spin-wave approach without (SW) and with (SWF) introducing Fermi operators (see (3)) are presented for comparison. On the inset the temperature dependence of the impurity site magnetization \bar{S}_0 at $H_A/J = 10^{-3}$, $J'/J = 0.15$ (solid line), $H_A/J = 10^{-3}$, $J'/J = 0.05$ (short-dashed line), $H_A/J = 10^{-2}$, $J'/J = 0.15$ (long-dashed line).

Fig.3 The temperature dependence of the short-range order parameters ξ, ξ' (solid lines, left scale) and correlation function $K = \langle \mathbf{S}_0 \mathbf{S}_\delta \rangle$ (dashed line, right scale) for the same parameter values as in Fig.2. Arrow shows the value of the Curie temperature.

Fig.4. The distribution of magnetization around impurity for the same parameter values as in Fig.2, $T = 0.3J$. Arrows show the value of magnetization disturbance at the impurity site ($R = 0$).

Fig.5. The temperature dependence of the parameters ξ, ξ' and spin correlation function $K = \langle \mathbf{S}_0 \mathbf{S}_\delta \rangle$ in the isotropic 2D ferromagnet with $S = S' = 1/2$, $J'/J = 0.15$. For comparison, the corresponding short-range order parameter in the ideal crystal, ξ_M , is shown.

Fig.6. The temperature dependence of the magnetizations for impurity site \bar{S}_0 , and for nearest-neighbor sites \bar{S}_1 in the case of antiferromagnetic impurity in the ferromagnetic host with $S = S' = 1/2$, $H_A/J = 10^{-3}$, $J'/J = -0.15$.

Fig.7. The temperature dependence of the magnetizations for impurity site \bar{S}_0 , and for nearest-neighbor sites \bar{S}_1 in the case of antiferromagnetic impurity in the ferromagnetic host with $S = S' = 1/2$, $H_A/J = 10^{-3}$, $J'/J = -1$.

Fig.8. The distribution of magnetization around antiferromagnetic impurity in the 2D isotropic ferromagnet at $T = 0$, $J'/J = 0.15$ (solid line), $J'/J = 0.05$ (dashed line).

Fig.9. The temperature dependence of magnetizations for impurity site \bar{S}_0 , and for nearest-neighbor sites \bar{S}_1 , in an antiferromagnet with $S = S' = 1/2$, $H_A/J = 10^{-3}$, $J'/J = 0.15$. Dashed lines show the corresponding results for a ferromagnet (Fig.2).

Fig.10. The temperature dependence of the short-range order parameters ξ, ξ' and correlation function $K = -\langle \mathbf{S}_0 \mathbf{S}_\delta \rangle$ for the same parameter values as in Fig.9. Arrow shows the value of the Neel temperature.

Fig.11. The distribution of magnetization around impurity in the 2D isotropic antiferromagnet at $T = 0$. The inset shows the picture at large R .

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